Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bis(4-methylpyridine-κN)-cobalt(II)]-di-μ-dicyanamido-$\kappa^2N^1:N^5$]

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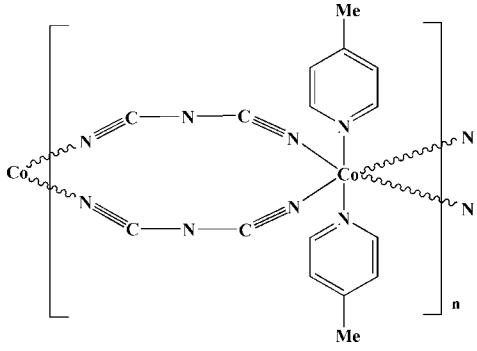
Received 5 December 2012; accepted 19 December 2012

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.085; data-to-parameter ratio = 13.5.

Cobalt(II) nitrate hexahydrate and sodium dicyanamide self-assembled in dimethylformamide (DMF) and 4-methylpyridine solutions to form the title compound, $[Co(C_2N_3)_2(C_6H_7N)_2]_n$. The Co^{2+} ion lies on an inversion center and adopts an octahedral coordination geometry in which four N atoms from four different dicyanamide ligands lie in the equatorial plane and two 4-methylpyridine N atoms occupy the axial positions. The Co^{II} atoms are connected by two bridging dicyanamide ligands, resulting in a chain parallel to the c axis. The chains are connected into a three-dimensional network by C—H···N hydrogen bonds.

Related literature

The design and syntheses of metal-organic compounds has attracted great attention not only as a result of their intriguing architectures and topologies (Eddaoudi *et al.*, 2001), but also because of their potential applications (Banerjee *et al.*, 2008).



Experimental

Crystal data

$[Co(C_2N_3)_2(C_6H_7N)_2]$
M_r = 377.28
Monoclinic, $P2_1/c$
a = 9.3686 (19) Å
b = 13.080 (3) Å
c = 7.3048 (15) Å
β = 106.86 (3)°
V = 856.7 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 150 K
0.21 × 0.17 × 0.15 mm

Data collection

Rigaku Saturn724+ diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
T_{min} = 0.815, T_{max} = 1.000
4994 measured reflections
1549 independent reflections
1419 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
S = 1.07
1549 reflections
115 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···N3^{i}	0.93	2.57	3.487 (3)	168

Symmetry code: (i) $-x+1, -y, -z+1$.

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation of China (No. 50472048) and the Program for New Century Excellent Talents in Universities (NCET-05–0499).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5034).

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supplementary materials

Acta Cryst. (2013). E**69**, m90 [doi:10.1107/S1600536812051252]

catena-Poly[[bis(4-methylpyridine-κN)cobalt(II)]-di-μ-dicyanamido-$\kappa^2N^1:N^5$]

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Comment

The design and syntheses of metal-organic compounds have attracted great attention in recent years because of not only their intriguing architectures and topologies (Eddaoudi *et al.*, 2001) but also their potential applications (Banerjee *et al.*, 2008). The title compound $\{Co[N(CN)_2]_2(NC_6H_7)_2\}_n$ is constructed by the flexible dicyanamide bridging ligands through diffusion reaction.

As illustrated in Fig. 1, Co^{2+} ion lies on an inversion center and adopts an octahedral coordination geometry, where four N atoms from four different dicyanamide ligands lie in the equatorial plane and two 4-methylpyridine N atoms occupy the axial positions. The Co atoms are connected by two dicyanamide ligands, resulting in a neutral chain along the *c*-axis. In the crystal, the chains are linked by C—H···N hydrogen bonds (Table 1) into a three-dimensional network.

Experimental

$Co(NO_3)_2?6H_2O$ (116.6 mg, 0.4 mmol) was added into 1 ml dmf with thorough stir for 5 minutes. After filtration, the purple filtrate was carefully laid on the surface with the solution of $NaN(CN)_2$ (89.1 mg, 1 mmol) in 1 ml dmf, 1 ml 4-methylpyridine and 5 ml *i*-PrOH. Pink block crystals were obtained after two weeks.

Refinement

H atoms were positioned geometrically and refined with riding model, with $U_{iso} = 1.5U_{eq}$ and $1.2U_{eq}$ for methyl and pyridyl H atoms, respectively. The C—H bonds are 0.96 Å in methyl and 0.93 Å in pyridyl.

Computing details

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear* (Rigaku, 2008); data reduction: *CrystalClear* (Rigaku, 2008); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

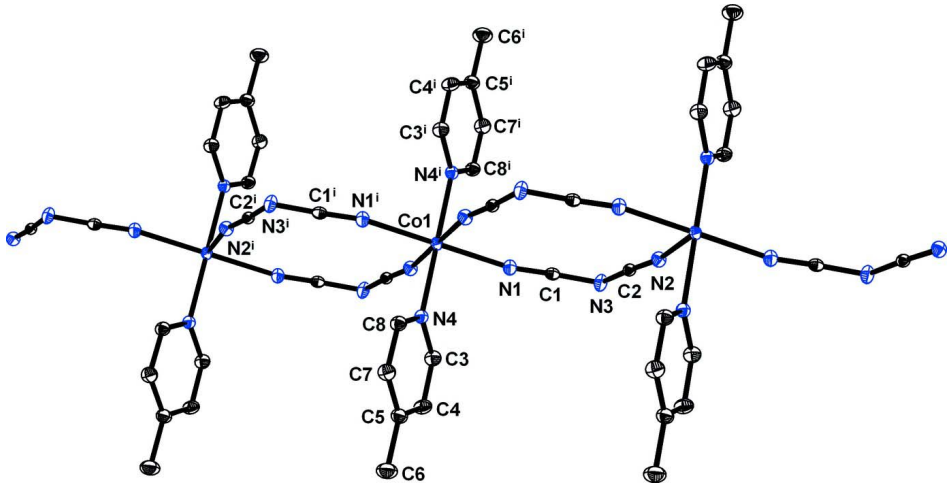

Figure 1

Portion of the polymeric chain of the title compound, with 30% probability displacement ellipsoids. All H atoms have been omitted. Symmetry code: (i) 2-x, -y, 1-z.

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Crystal data

$[Co(C_2N_3)_2(C_6H_7N)_2]$
$M_r = 377.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.3686$ (19) Å
$b = 13.080$ (3) Å
$c = 7.3048$ (15) Å
$\beta = 106.86$ (3)°
$V = 856.7$ (3) Å^3
$Z = 2$
$F(000) = 386$
$D_x = 1.463$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3521 reflections
$\theta = 3.1$–$28.7°$
$\mu = 1.02$ mm^{-1}
$T = 150$ K
Block, pink
0.21 × 0.17 × 0.15 mm

Data collection

Rigaku Saturn724+ diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
$T_{min} = 0.815$, $T_{max} = 1.000$
4994 measured reflections
1549 independent reflections
1419 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 25.4°$, $\theta_{min} = 3.3°$
$h = -10 \rightarrow 11$
$k = -12 \rightarrow 15$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.085$
$S = 1.07$
1549 reflections
115 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.6117P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	1.0000	0.0000	0.5000	0.01854 (16)
N1	0.86523 (19)	−0.07208 (14)	0.6510 (3)	0.0262 (4)
N2	0.87457 (19)	−0.07142 (14)	1.2428 (2)	0.0249 (4)
N3	0.76592 (19)	−0.12944 (15)	0.9113 (2)	0.0275 (4)
N4	0.85008 (18)	0.12713 (13)	0.4394 (2)	0.0213 (4)
C1	0.8228 (2)	−0.09665 (15)	0.7775 (3)	0.0203 (4)
C2	0.8276 (2)	−0.09642 (15)	1.0853 (3)	0.0194 (4)
C3	0.7023 (2)	0.11338 (17)	0.3732 (3)	0.0274 (5)
H3B	0.6656	0.0469	0.3562	0.033*
C4	0.6022 (2)	0.19299 (18)	0.3293 (3)	0.0315 (5)
H4A	0.5006	0.1796	0.2828	0.038*
C5	0.6525 (2)	0.29340 (17)	0.3544 (3)	0.0287 (5)
C6	0.5461 (3)	0.3821 (2)	0.3074 (4)	0.0420 (6)
H6A	0.4458	0.3570	0.2615	0.063*
H6B	0.5682	0.4235	0.2105	0.063*
H6C	0.5566	0.4225	0.4203	0.063*
C7	0.8053 (2)	0.30713 (17)	0.4229 (3)	0.0301 (5)
H7A	0.8448	0.3728	0.4420	0.036*
C8	0.8989 (2)	0.22389 (16)	0.4628 (3)	0.0261 (5)
H8A	1.0010	0.2353	0.5083	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0207 (2)	0.0195 (2)	0.0153 (2)	−0.00038 (14)	0.00501 (16)	−0.00061 (14)
N1	0.0278 (9)	0.0278 (10)	0.0236 (9)	−0.0027 (7)	0.0086 (8)	0.0009 (8)
N2	0.0263 (9)	0.0267 (9)	0.0206 (10)	−0.0019 (7)	0.0053 (7)	−0.0036 (7)
N3	0.0242 (9)	0.0401 (11)	0.0181 (9)	−0.0131 (8)	0.0059 (7)	−0.0038 (8)
N4	0.0218 (8)	0.0219 (9)	0.0198 (9)	−0.0009 (7)	0.0053 (7)	−0.0008 (7)
C1	0.0169 (9)	0.0205 (10)	0.0201 (10)	−0.0007 (7)	0.0001 (8)	−0.0034 (8)
C2	0.0167 (9)	0.0191 (9)	0.0227 (11)	−0.0006 (7)	0.0064 (8)	0.0021 (8)
C3	0.0241 (10)	0.0258 (11)	0.0309 (12)	−0.0044 (8)	0.0056 (9)	−0.0032 (9)
C4	0.0193 (10)	0.0349 (12)	0.0386 (13)	−0.0010 (9)	0.0055 (9)	−0.0012 (10)
C5	0.0285 (11)	0.0283 (12)	0.0285 (11)	0.0055 (9)	0.0072 (9)	0.0017 (9)
C6	0.0370 (13)	0.0372 (14)	0.0511 (16)	0.0127 (11)	0.0118 (12)	0.0034 (12)
C7	0.0309 (11)	0.0213 (11)	0.0382 (13)	−0.0014 (9)	0.0102 (10)	−0.0010 (9)
C8	0.0217 (10)	0.0250 (11)	0.0306 (12)	−0.0024 (8)	0.0062 (9)	−0.0005 (9)

Geometric parameters (Å, º)

Co1—N2^{i}	2.1219 (18)	C3—C4	1.376 (3)
Co1—N2^{ii}	2.1219 (18)	C3—H3B	0.9300
Co1—N1^{iii}	2.1229 (18)	C4—C5	1.389 (3)
Co1—N1	2.1229 (18)	C4—H4A	0.9300
Co1—N4	2.1385 (17)	C5—C7	1.384 (3)
Co1—N4^{iii}	2.1385 (17)	C5—C6	1.503 (3)
N1—C1	1.152 (3)	C6—H6A	0.9600
N2—C2	1.153 (3)	C6—H6B	0.9600
N2—Co1^{iv}	2.1219 (18)	C6—H6C	0.9600
N3—C2	1.308 (3)	C7—C8	1.375 (3)
N3—C1	1.314 (3)	C7—H7A	0.9300
N4—C8	1.340 (3)	C8—H8A	0.9300
N4—C3	1.340 (3)		
N2^{i}—Co1—N2^{ii}	180.00 (7)	N2—C2—N3	175.1 (2)
N2^{i}—Co1—N1^{iii}	89.76 (7)	N4—C3—C4	123.1 (2)
N2^{ii}—Co1—N1^{iii}	90.24 (7)	N4—C3—H3B	118.5
N2^{i}—Co1—N1	90.24 (7)	C4—C3—H3B	118.5
N2^{ii}—Co1—N1	89.76 (7)	C3—C4—C5	120.2 (2)
N1^{iii}—Co1—N1	180.00 (9)	C3—C4—H4A	119.9
N2^{i}—Co1—N4	89.84 (7)	C5—C4—H4A	119.9
N2^{ii}—Co1—N4	90.16 (7)	C7—C5—C4	116.5 (2)
N1^{iii}—Co1—N4	90.06 (7)	C7—C5—C6	122.0 (2)
N1—Co1—N4	89.94 (7)	C4—C5—C6	121.5 (2)
N2^{i}—Co1—N4^{iii}	90.16 (7)	C5—C6—H6A	109.5
N2^{ii}—Co1—N4^{iii}	89.84 (7)	C5—C6—H6B	109.5
N1^{iii}—Co1—N4^{iii}	89.94 (7)	H6A—C6—H6B	109.5
N1—Co1—N4^{iii}	90.06 (7)	C5—C6—H6C	109.5
N4—Co1—N4^{iii}	180.0	H6A—C6—H6C	109.5
C1—N1—Co1	159.33 (16)	H6B—C6—H6C	109.5
C2—N2—Co1^{iv}	163.96 (16)	C8—C7—C5	120.2 (2)
C2—N3—C1	117.09 (17)	C8—C7—H7A	119.9
C8—N4—C3	116.84 (18)	C5—C7—H7A	119.9
C8—N4—Co1	121.94 (13)	N4—C8—C7	123.2 (2)
C3—N4—Co1	121.22 (14)	N4—C8—H8A	118.4
N1—C1—N3	175.1 (2)	C7—C8—H8A	118.4

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) −*x*+2, −*y*, −*z*+2; (iii) −*x*+2, −*y*, −*z*+1; (iv) *x*, *y*, *z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···N3^{v}	0.93	2.57	3.487 (3)	168

Symmetry code: (v) −*x*+1, −*y*, −*z*+1.